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# Detection of Nanoscale Soil Organic Matter by Middle Infrared Spectrum for Forensic Science

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**Abstract** Soil is useful as a kind of trace evidence for forensic science. Thus it is very crucial to identify sources of soil. The nanoscale soil organic matter (NSOMs) can be used to differentiate soil sources because their constituents and contents are relatively stable with time but variant by location. In this study, NSOMs from eighteen regions of Shandong Province in China were examined by middle infrared spectrum (4000–400 cm<sup>-1</sup>). The results showed that the constituents and contents of NSOMs in eighteen samples were dramatically different; a NSOM fingerprint for each sample was drawn based on these characteristics. This suggests that a national or global NSOM fingerprint database could be rapidly established by the one-step middle infrared spectrum analysis for different soil samples, which will be helpful to determine crime scenes by comparing the middle infrared spectrum of forensic soil with the NSOMs fingerprint database.

**Keywords:** Forensic science, Middle Infrared Spectrum, Nanoscale Soil Organic Matter.

## 1 Introduction

Soil as important trace evidence can provide meaningful information for criminal investigation. The constituents of soil consist of organic matter, inorganic mineral grain, chemical precipitates (such as calcium carbonate and salt crystal), dead plants, animal matter, insect carapace, bacteria, soil algae, fungi, roots of higher plants, and so forth. Forensic detection of soil evidence has been performed by comparing soil components like organic matter, heavy and light minerals, oxides, stable and radioactive isotopes, pollens, diatoms, and microorganisms, meanwhile determining physical properties, such as color, distribution of particle sizes, and density<sup>[1]</sup>. Of these characteristics, the nanoscale soil organic matter (NSOMs) are the most easily affected by environmental factors, for instance, weathering, microorganisms present in the soil,

plants in nearby soil, animal residues, and artifacts of human beings<sup>[2]</sup>. This means soil from different places was discrepant. However, NSOMs are relatively stable in a period, which may give actual information from crime scenes.

The main constituents of NSOMs were composed of lignin, lipid or fatty acid, carbohydrate, protein, cellulose, hopane, and so forth<sup>[3]</sup>. The main functional groups of these compounds can be rapidly identified and quantified by middle infrared spectrum (4000–400 cm<sup>-1</sup>), which has become a powerful rapid assessment tool for determining soil properties<sup>[4]</sup>. In this study, eighteen soil samples from different regions in Shandong Province in China were selected and applied to Fourier transform infrared spectroscopy. Their NSOMs constituents (the main functional groups) and contents were rapidly and accurately determined. The results showed that there was a

one-to-one relationship between the constituents and contents of NSOMs and the soil sources. Thus, a NSOM fingerprint was easily drawn, which suggests that it is possible to perform the rapid batch detections for a large number of soil samples to establish a national or global NSOM fingerprint database for forensic science.

## 2 Materials and Methods

**2.1. Sample Collection.** Eighteen soil samples were collected from different regions in Shandong Province in China. Samples were named as S1 to S18, representing Heze, Qufu, Zibo, Zhuangjia (Yantai), Penglai (Yantai), Zouping County (Bingzhou), Jiexiang County (Jining), Kenli County (Dongying), Wulian County (Rizhao), Zaozhuang, Laiwu, Liaocheng, Rongcheng (Weihai), Jiaozhou (Qingdao), South Mountainous Area (Jinan), Taian, Changyi (Weifang),

Xiajin (Dezhou), and Jining, respectively.

**2.2. Sample Preparation.** Soil samples were ground down into powder and dried at 120°C for 12 hours. Then 2.5 mg of the dried soil sample was mixed with 500 mg of dry potassium bromide (KBr). The mixture was pressed into a mold (8 mm in diameter and 0.05 mm in thickness) with a pressure of  $1 \times 10^8$  kg/m<sup>2</sup>.

**2.3. Infrared Spectra.** Infrared spectra were recorded in frequency ranges from 4000 to 400 cm<sup>-1</sup> by a Fourier transform infrared spectroscopy (Bruker AXS VERTEX 70, Germany). The quantitative analysis of NSOMs was performed using KBr tablet method according to JJG-1996.

### 3 Results and Discussion

**3.1. The Organic Spectra Peak Assignment.** According to the previous investigation about the infrared spectra of soil organic matter (SOMs)<sup>[4-7]</sup>, the peak assignments from S1 to S18 were analyzed. As shown in Figure 1, the peak assignment was varied with the soil source. The wide absorption peaks at 3591–3626 cm<sup>-1</sup> were the characteristics of hydroxyl groups (–OH). The small peaks at 3107–3448 cm<sup>-1</sup> and 2322–2360 cm<sup>-1</sup> were the characteristics of –NH and NH<sup>+</sup>, respectively. The peaks at 1612–1616 cm<sup>-1</sup> belonged to C=C stretching. The peaks at 1429–1635 cm<sup>-1</sup> were attributed to O–N=O/C=C stretching. The peaks at 1379–1436 cm<sup>-1</sup> were assigned to C–N=O/C=O stretching. The broad and intense stretching peaks at 1379–1384 cm<sup>-1</sup> belonged to C–H stretching. The peaks at 1006–1122 cm<sup>-1</sup> were assigned to C–O stretching. The peaks at 1000–1100 cm<sup>-1</sup> and 1014–1024 cm<sup>-1</sup> belonged to the characteristics of P–O–R and C–O–C/C–O, respectively. The peaks at 740–779 cm<sup>-1</sup> were associated with C–O–C or C–H stretching vibrations. The strong stretching peaks at 484–532 cm<sup>-1</sup> and 469–457 cm<sup>-1</sup> were attributed to P–Cl and C–X (halogen) stretching,

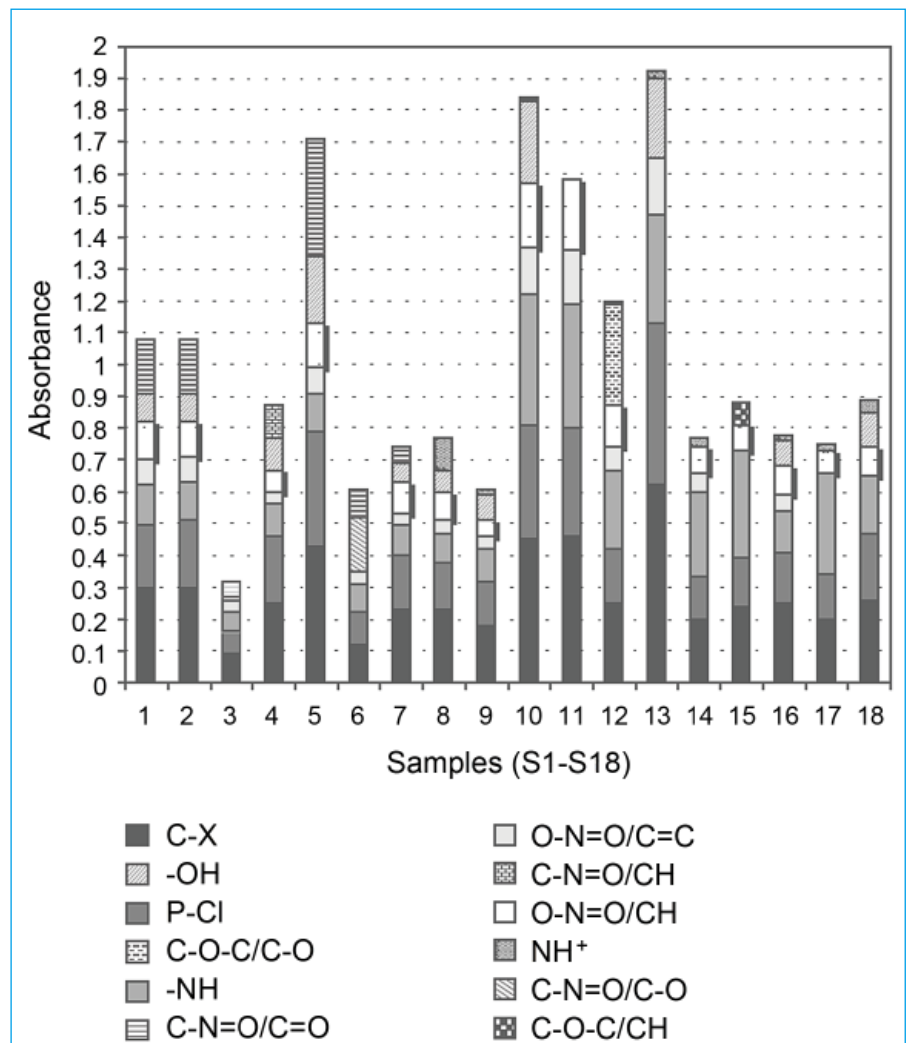


Figure 1. Infrared spectra of eighteen soil samples (S1 to S18).

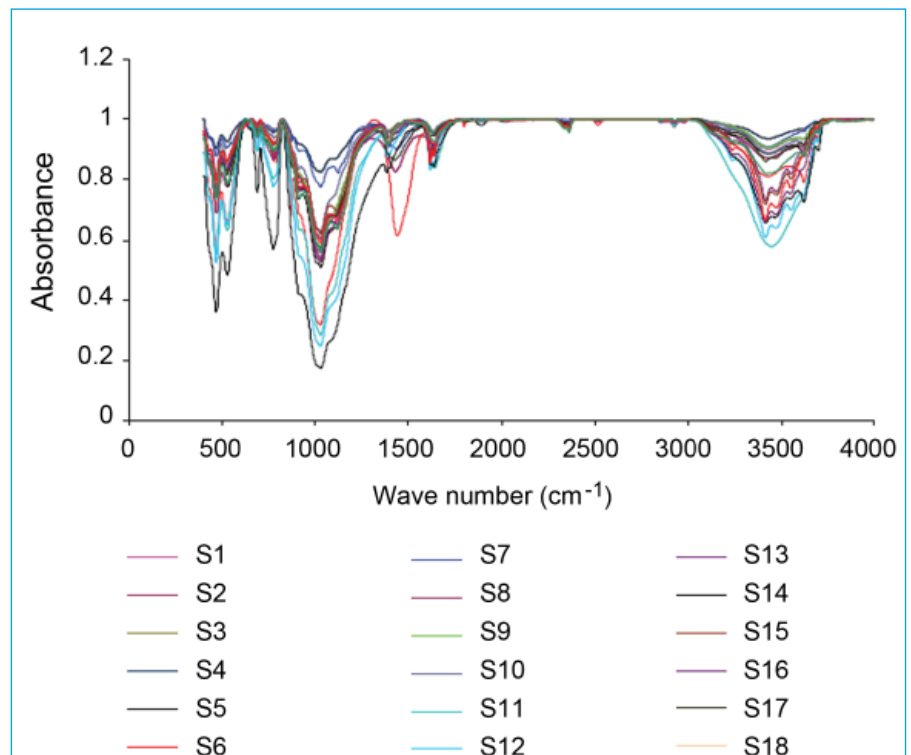


Figure 2. The number, type, and absorbance value of the main functional groups in NSOMs.

respectively.

### 3.2. Quantitative Analysis.

The numbers and types of the main functional groups in NSOMs of S1–S18 were analyzed according to the infrared data. As shown in Figure 2, the number, type, and absorbance value of the main functional groups in NSOMs varied with the source of the soil sample due to a variety of geological environments in different regions. The samples S1, S2, S4, S5, S7, S8, S9, S10, and S12 were composed of seven functional groups. S6, S13, and S18 consisted of six functional groups. S3, S11, S14, S15, and S17 contained five functional groups.

The hydroxyl group (–OH) was present in all of 18 samples, but it was infinitesimal in S6, S15, S16, and S17. There were eleven types of functional groups in S18, which indicated that this sample contained abundant organic matter<sup>[8]</sup>. By contrast, S11 and S15 only contained seven types of functional groups, which suggested that the organic matter were poor in these soil samples. The relative contents of C–X and P–Cl groups in S13 were highest in all of the samples, which were probably associated with the situated chemical plants in the sampling locations<sup>[9]</sup>. However, there were scarcely any C–X and P–Cl groups in S3, which meant that the soil of the sampling location was hardly contaminated<sup>[10]</sup>.

The types of the main functional groups were only halfway similar for each sample. The absorbance value of the same functional group was different as well. These differences will be a favorable reference for the analysis of the soil source using a computer program.

Table 1. The database table design of S1 sample.

Number of functional groups	Type of functional groups	Absorbance value of functional groups
7	C–X	0.31
	P–Cl	0.19
	–NH	0.13
	O–N=O/C=C	0.09
	O–N=O/CH	0.12
	C–N=O/C–O	0.08
	–OH	0.17

### 3.3. NSOM Fingerprint

**Database.** The SOM fingerprint database of tested soil samples (S1–S18) could be established according to the difference of the main functional groups in SOMs identified by the middle infrared spectra. The scheme of SOM fingerprint database was designed as follows: the database was created and named as A. Then a table, namely B, was created in this directory, which contained some fields including number, type, and absorbance value of the main functional groups of NSOMs in each soil sample. Taking the table of S1 sample as an example, the procedure of the database table design was described (Table 1). Thus, the source of unknown soil sample may be rapidly identified using computer program through an SQL main organic functional groups query (SELECT \* FROM TABLE B WHERE B.NumberOfKind = sample's number of kind AND B.Absorbance valueOf type1 = sample's concent of type1 AND. . .). This suggests that the establishment of the forensic SOM fingerprint database was feasible based on the infrared spectra analysis of SOMs, and the crime scenes will be rapidly locked using the forensic SOM fingerprint database.

## 4 Conclusions

In this study, Fourier transform middle infrared spectroscopy was applied to analyze eighteen soil samples from different regions of Shandong Province in China. The resulting infrared spectra showed that the constituents and contents of nanoscale soil organic matter (NSOMs) were varied with their sources.

The main NSOM constituents of tested samples were composed of –OH, –NH, NH<sup>+</sup>, C=C, O–N=O/C=O, C–N=O/C=O, C–H, C–O, P–O=R, C–O–C, O–N=O/CH, P–Cl, and C–X with different contents. Based on these characteristics, the NSOM fingerprints of tested soil samples were established, which could be useful for the rapid analysis of crime scenes by comparing the forensic soil with the NSOM fingerprint database.

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